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Contents

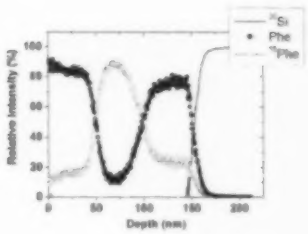
Regular Articles

1–7

Molecular depth profiling of model biological films using low energy monoatomic ions

J. Brison, N. Mine, N. Wehbe, X. Gillon, T. Tabarrant, R. Sporken, L. Houssiau

► We report a systematic study of ToF-SIMS depth profiling performance on model biological samples. ► Amino acid and nucleoside layers were deposited on silicon wafers using vacuum thermal evaporation. ► Low energy monatomic primary ions were used as primary ions for depth profiling. ► Complex multi-layers were also investigated.

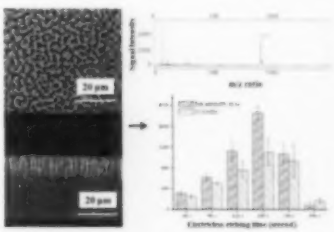


8–13

Preparation of nanostructured silicon surface for mass spectrometry analysis by an all-wet fabrication process using electroless metal deposition and metal assisted etching

Chia-Wen Tsao, Zhi-Jie Yang, Cheng-Wei Chung

► A simple low-cost high-throughput all-wet fabrication process to create silicon nanostructure for mass spectrometry analysis is proposed. ► Electroless deposition and etching time effects are discussed. ► 150 s electroless deposition and 180 s etching time show highest mass spectrometry detection sensitivity. ► Silicon nanostructure surface assisted mass spectrometry can be used at lower fabrication cost and higher production throughput.

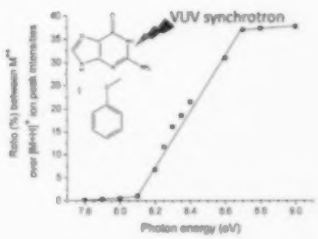


14–18

Atmospheric pressure photoionization mass spectrometry of guanine using tunable synchrotron VUV radiation

Julie Allegrand, David Touboul, Alexandre Giuliani, Alain Brunelle, Olivier Laprévote

► First experiments coupling a commercial APPI source with a synchrotron radiation facility. ► Without dopant: linear increase of the $[M+H]^+$ ion from guanine for energy greater than 8.2 eV. ► With anisole as a dopant: appearance of a radical cation $M^{\bullet+}$. ► Increase of the $M^{\bullet+}/[M+H]^+$ ratio between 8.2 and 8.7 eV. ► Ionization mechanisms imply direct photoionization, proton and charge transfers.



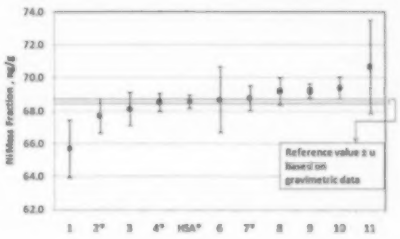
Elsevier B.V.
http://dx.doi.org/10.1016/S1387-3806(12)00240-0

19–24

High accuracy measurements of trace elements in drinking water by exact matching isotope dilution mass spectrometry (IDMS)

Sin Yee Ng, Aimei Zou, Lay Peng Sim, Yi Ding, Kim Loong Yuen, Richard Y.C. Shin, Tong Kooi Lee

► Exact-matching isotope dilution mass spectrometry was used for the analysis of trace elements in drinking water. ► High accuracy results traceable to the International System of Units (SI) were obtained. ► An expanded uncertainty with less than 2% combined uncertainty ($\kappa = 2$) were achieved for all analytes.

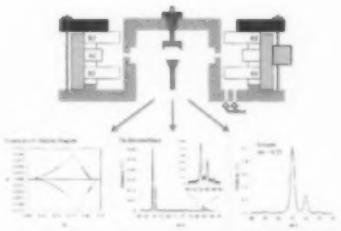


25–32

A simplified toroidal ion trap mass analyzer

Nicholas Taylor, Daniel E. Austin

► A toroidal ion trap mass analyzer utilizing cylindrical electrodes is presented. ► Resolution of toluene *m/z* 91 is evaluated for both scan direction and higher order multipole components. ► Optimal parameters yield resolution values superior to previously reported toroidal designs. ► The first stability diagram of an ion trap with a toroidal trapping geometry is presented and discussed. ► Tandem (MS^2) mass spectrometry of iso-butylbenzene is demonstrated.

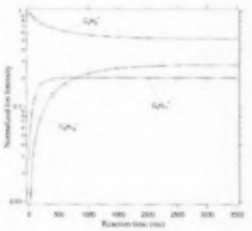


33–39

Gas-phase ion–molecule reactions in selected cyclohexanes

C.Q. Jiao, S.F. Adams

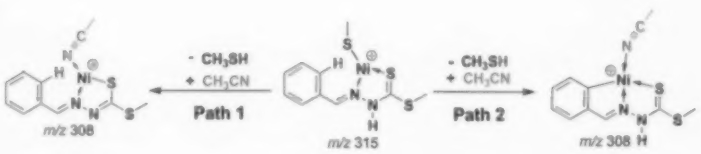
► Ion reactions in cyclohexane, methylcyclohexane and ethylcyclohexane were studied. ► Reactions take place mainly via charge transfer, H^- transfer and $H2^-$ transfer. ► Most reactions proceed in a direct mode. ► There is evidence of structural isomers for certain hydrocarbon reactant ions.



40–48

Electrospray mass spectrometric studies of nickel(II)-thiosemicarbazones complexes: Intra-complex proton transfer in the gas phase ligand exchange reactions

Kezhi Jiang, Gaofeng Bian, Yunfeng Chai, Huameng Yang, Quoqiao Lai, Yuanjiang Pan

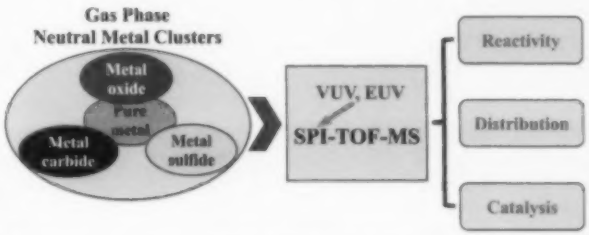


Review Article

49–65

Gas phase chemistry of neutral metal clusters: Distribution, reactivity and catalysis

Shi Yin, Elliot R. Bernstein



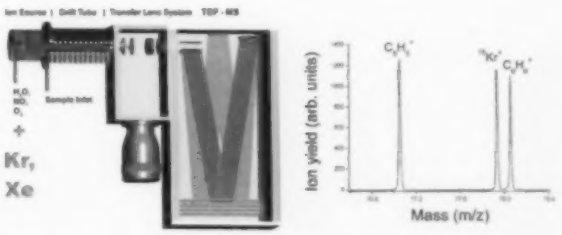
▶ Recent work on gas phase distribution, reactivity, and catalysis of neutral metal clusters investigated by SPI-TOFMS is reviewed. ▶ The reactivity of metal oxide clusters is associated with their oxygen-rich or -deficient nature, bond enthalpy, and unpaired spin density. ▶ The catalytic activity of metal clusters for bond activation catalysis is dependent up on their association and activation capabilities. ▶ Insights into how application of neutral metal cluster chemistry is instructive in understanding of important fundamental aspects of practical catalysis are provided.

Short Communications

66–70

From conventional proton-transfer-reaction mass spectrometry (PTR-MS) to universal trace gas analysis

Philipp Sulzer, Achim Edtbauer, Eugen Hartungen, Simone Jürschik, Alfons Jordan, Gernot Hanel, Stefan Feil, Stefan Jaksch, Lukas Märk, Tilmann D. Märk

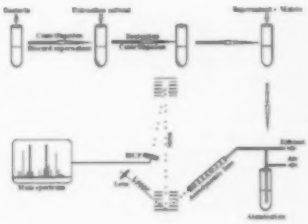


▶ Kr+ is introduced as a reagent ion in conventional PTR-MS for the very first time. ▶ We greatly extended the analyzable substance classes to important molecules such as CO, CO_2, CH_4, NO_x, and SO_2, etc. ▶ No major changes in instrumental setup in order to access these additional substance classes. ▶ We achieve a reagent ion purity of over 93% and nearly 9×10^6 cps reagent ion signal. ▶ The high mass resolution allows for the separation of all isobaric compounds in the present study.

71–76

Rapid lipid profiling of bacteria by online MALDI-TOF mass spectrometry

Xi Shu, Yueyan Li, Miao Liang, Bo Yang, Changgeng Liu, Youfeng Wang, Jinian Shu



▶ Online droplet-deposited MALDI mass spectrometer is applied to detect bacteria. ▶ Characteristic lipid profiling of three bacteria are obtained. ▶ The present technique is capable of conducting rapid lipid analysis and has the potential for rapid bioaerosol detection.

Erratum

77–77

Erratum to "Dissociative electron attachment to the silane derivatives trichlorovinylsilane ($SiCl_3C_2H_3$), tetravinylsilane ($Si(C_2H_3)_4$) and trimethylvinylsilane ($Si(CH_3)_3C_2H_3$)" [Int. J. Mass Spectrom. 315 (2012) 40–45]

Jaroslav Kočišek, Eugen Illenberger, Štefan Matejčík